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NEWS 4	AUG 24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS 5	AUG 24	CA/CAplus enhanced with legal status information for U.S. patents
NEWS 6	SEP 09	50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS 7	SEP 11	WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus
NEWS 8	OCT 21	Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded
NEWS 9	OCT 21	Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models
NEWS 10	NOV 23	Addition of SCAN format to selected STN databases
NEWS 11	NOV 23	Annual Reload of IFI Databases
NEWS 12	DEC 01	FRFULL Content and Search Enhancements
NEWS 13	DEC 01	DGENE, USGENE, and PCTGEN: new percent identity feature for sorting BLAST answer sets
NEWS 14	DEC 02	Derwent World Patent Index: Japanese FI-TERM thesaurus added
NEWS 15	DEC 02	PCTGEN enhanced with patent family and legal status display data from INPADOCDB
NEWS 16	DEC 02	USGENE: Enhanced coverage of bibliographic and sequence information
NEWS 17	DEC 21	New Indicator Identifies Multiple Basic Patent Records Containing Equivalent Chemical Indexing in CA/CAplus
NEWS 18	JAN 12	Match STN Content and Features to Your Information Needs, Quickly and Conveniently

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AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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FILE 'HOME' ENTERED AT 13:45:08 ON 20 JAN 2010

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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FILE 'REGISTRY' ENTERED AT 13:45:19 ON 20 JAN 2010
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STRUCTURE FILE UPDATES: 19 JAN 2010 HIGHEST RN 1202629-39-7
DICTIONARY FILE UPDATES: 19 JAN 2010 HIGHEST RN 1202629-39-7

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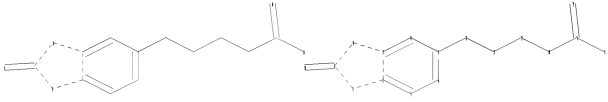
Uploading C:\Program Files\STNEXP\Queries\10517264c.str



chain nodes :
10 11 12 13 14 15 16 17
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
5-11 8-10 11-12 12-13 13-14 14-15 15-16 15-17
ring bonds :

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1-2  1-6  2-3  2-7  3-4  3-9  4-5  5-6  7-8  8-9
exact/norm bonds :
2-3  2-7  3-9  7-8  8-9  8-10  15-16  15-17
exact bonds :
5-11  11-12  12-13  13-14  14-15
normalized bonds :
1-2  1-6  3-4  4-5  5-6


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS



L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
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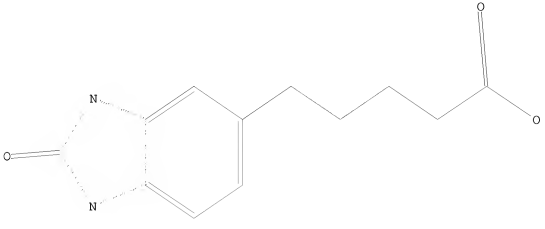


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Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 13:45:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      161 TO ITERATE

100.0% PROCESSED      161 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:          2459 TO     3981
PROJECTED ANSWERS:                1 TO       80

L2            1 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 13:45:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2934 TO ITERATE

100.0% PROCESSED     2934 ITERATIONS                               15 ANSWERS
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SEARCH TIME: 00.00.01

L3 15 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 191.54 191.76

FILE 'CAPLUS' ENTERED AT 13:45:41 ON 20 JAN 2010
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FILE COVERS 1907 - 20 Jan 2010 VOL 152 ISS 4
FILE LAST UPDATED: 19 Jan 2010 (20100119/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

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http://www.cas.org/legal/infopolicy.html

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=> s l4
L4 NOT FOUND
The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> s l3
L4 6 L3

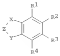
=> d ibib abs hitstr tot

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:991486 CAPLUS
DOCUMENT NUMBER: 140:27827
TITLE: Preparation of benzimidazole derivatives which inhibit the cytokine or biological activity of macrophage migration inhibitory factor (MIF)
INVENTOR(S): Morand, Eric Francis; Iskander, Magdy Naguib
PATENT ASSIGNEE(S): Cortical Pty. Ltd., Australia
SOURCE: PCT Int. Appl., 149 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003104203	A1	20031218	WO 2003-AU717		20030606
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2487838	A1	20031218	CA 2003-2487838		20030606
AU 2003233244	A1	20031222	AU 2003-233244		20030606
GB 2405147	A	20050223	GB 2004-27242		20030606
GB 2405147	B	20061122			
EP 1511736	A1	20050309	EP 2003-727010		20030606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
CN 1675185	A	20050928	CN 2003-818935		20030606
JP 2005533049	T	20051104	JP 2004-511273		20030606
NZ 537301	A	20060630	NZ 2003-537301		20030606
IN 2004KN01848	A	20060804	IN 2004-KN1848		20041206
ZA 2004009845	A	20060927	ZA 2004-9845		20041206
US 20060154977	A1	20060713	US 2005-517264		20050930
PRIORITY APPLN. INFO.:			AU 2002-2832	A	20020607
			AU 2002-2834	A	20020607
			WO 2003-AU717	W	20030606

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 140:27827
GI

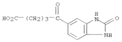


I

AB Title compds. I [X = O, S, alkyl, amino; Y = amino, O, S, alkyl; Z = CO, CS, imino, SO, SO_2; R1 = H, alkyl, alkyloxy, etc.; R2 = alkyl, alkenyl, alkynyl, etc.; R3 = H, alkyl, alkylamino, alkylalkoxy, etc.; R4 = H, halo, alkyl, alkenyl, alkynyl, etc.] are prepared For instance, 3,4-diaminotoluene is reacted with urea (pentanol, reflux) to give 5-methylbenzimidazol-2-one (56%). Example compds. are inhibitors of the cytokine or biol. activity of macrophage migration inhibitory factor (MIF). I are useful for the treatment of Lyme disease, connective tissue diseases, etc.

IT 36896-35-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted benzimidazoles which inhibit the cytokine or biol. activity of macrophage migration inhibitory factor (MIF))

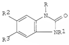
RN 36896-35-2 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-δ,2-dioxo- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1981:78266 CAPLUS
DOCUMENT NUMBER: 94:78266
ORIGINAL REFERENCE NO.: 94:12675a,12678a
TITLE: Antimetabolite properties of some benzimidazole derivatives and their fungicidal activity against the cotton wilt pathogen
AUTHOR(S): Kadyrov, Ch. Sh.; Kosyakovskaya, M. N.; Ayupova, A. T.; Molchanov, L. V.; Gordeeva, A. V.; Balikhina, V. N.; Filippov, V. V.
CORPORATE SOURCE: USSR
SOURCE: Fungitsidy (1980), 34-42. Editor(s): Mel'nikov, N. N.
Izd. Fan Uzb. SSR: Tashkent, USSR.
CODEN: 44UOAK
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI



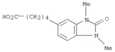
I, $R=R^1=R^2=H$, $R^3=CH_2CH_2CO_2H$
II, $R=R^1=Me$, $R^2=H$, $R^3=Cl$
III, $R=R^1=R^2=Me$, $R^3=(CH_2)_4CO_2H$
IV, $R=R^1=H$, $R^2=Cl$, $R^3=CH=CHCO_2H$
V, $R=CMe=CH_2$, $R^1=R^2=H$, $R^3=Cl$
VI, $R=R^1=R^2=H$, $R^3=Cl$

AB Benzimidazolonylpropionic acid (I) [76381-41-4] at 50 mg/L lowered the Saccharomyces cervisiae growth rate to 6% of controls and at 2.5 μg/L showed a weak biotin activity (4% of the activity of biotin). 5-Chloro-1,3-dimethylbenzimidazolene (II) [53439-90-0] stimulated yeast growth by 97% and showed in 80% biotin activity. 1,3-Dimethylbenzimidazolonylvalerionic acid [17767-91-8], 5-chloro-1,3-dimethylbenzimidazolonylvalerianic acid [76381-47-0], benzimidazolonylbutyric acid [6646-65-7], 5-methyl-1,3-dimethylbenzimidazolonylvaleric acid (III) [76381-42-5], and 5-methylbenzimidazolonylvalerionic acid [76381-48-1] stimulated the yeast growth as much as, or more than, did I, although their biotin activity was only 7-24%. Of 4 compds. showing antibiotin activity benzimidazolonoylacrylic acid [76381-38-9], N,N'-dimethylbenzimidazolanoylacrylic acid [32399-40-9], 5-methylbenzimidazolonoylacrylic acid [76381-39-0], and 5-chlorobenzimidazolonoylacrylic acid (IV) [76381-40-3] IV showed the highest antiwilt effect. Of 6 title compds., only 10 mg 5-chloro-N-isopropenylbenzimidazolone (V) [52125-61-8] and 5-chlorobenzimidazolone (VI) [2034-23-3]/L inhibited the growth of a pathogenic Verticillium dahliae strain to 60 and 13% of controls, resp., whereas 4 ethers stimulated the growth by 6-44%. V acted by disrupting the functions of B group vitamins and N-containing bases. Synthesis was given.

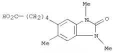
IT 17767-91-8P 76381-42-5P 76381-47-0P 76381-48-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and fungicidal and antimetabolite and antivitamin activity of)

RN 17767-91-8 CAPLUS

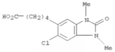
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-1,3-dimethyl-2-oxo- (CA INDEX NAME)



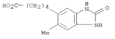
RN 76381-42-5 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-1,3,6-trimethyl-2-oxo- (CA INDEX NAME)



RN 76381-47-0 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 6-chloro-2,3-dihydro-1,3-dimethyl-2-oxo- (CA INDEX NAME)



RN 76381-48-1 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-6-methyl-2-oxo- (CA INDEX NAME)



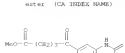
L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1972:461882 CAPLUS
DOCUMENT NUMBER: 77:61882
ORIGINAL REFERENCE NO.: 77:10239a,10242a
TITLE: Acylation of benzimidazolone and its derivatives by acid anhydrides and chlorides
AUTHOR(S): Kasyanovskaya, M. N.; Gordeeva, A. V.; Kadyrov, Ch. Sh.
CORPORATE SOURCE: Inst. Khim. Rast. Veshch., Tashkent, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (3), 386-9
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Acylation of benzimidazolones (I, R = R1 = H, Me) under Friedel-Crafts conditions with anhydrides gave II (n = 2,3) whereas uncatalyzed reaction of anhydrides with benzimidazolone gave III (R2 = Ac, BzCO, PrCO, ClCH2CO). BzCHCO; R3 = Me, NO2, Cl). Thus 0.03 mole I (R = R1 = H) was treated with 0.07 mole succinic anhydride in AlCl3-CH2Cl4 to give 92% II (R = R1 = H, n = 2), while reaction of I (R = R1 = H) with Ac2O in CCl4 gave 92% III (R3 = Ac, 14 = 0).
IT 36896-35-2P 36896-36-3P 36896-37-4P
36896-41-0P 36896-42-1P 36896-43-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36896-35-2 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-8,2-dioxo- (CA INDEX NAME)

RN 36896-36-3 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-1,3-dimethyl-8,2-dioxo- (CA INDEX NAME)

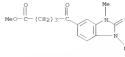
RN 36896-37-4 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-6-methyl-8,2-dioxo- (CA INDEX NAME)

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

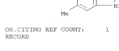
RN 36896-41-0 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-8,2-dioxo-, methyl ester (CA INDEX NAME)



RN 36896-42-1 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-1,3-dimethyl-8,2-dioxo-, methyl ester (CA INDEX NAME)

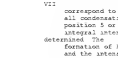


RN 36896-43-2 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-6-methyl-8,2-dioxo-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1967:477596 CAPLUS
DOCUMENT NUMBER: 67:77596
ORIGINAL REFERENCE NO.: 67:14633a,14634a
TITLE: Infrared spectra of some benzimidazolone derivatives
AUTHOR(S): Zaabkes, Ya. V.
SOURCE: Zhurnal Prikladnoi Spektroskopii (1967), 6(4), 505-10
CODEN: ZPSBAX; ISSN: 0514-7506
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Ir spectra of benzimidazolone (I), 1,3-dimethylbenzimidazolone (II), phenylbutyric acid (III), benzimidazolonylbutyric acid (IV), 1,3-dimethylbenzimidazolonylbutyric acid (V), γ-benzimidazolonylbutyric acid (VI), and of δ-benzimidazolonylvaleric acid (VII) were measured in pyridine and in KBr pellets. The character of the products obtained by the condensation of I or II with γ-butyrolactone and with δ-valerolactone in the presence of anhydrous AlCl3 (the position of alkyl substitution in the benzene ring, H bond association) was thus investigated. Bands at 808-817 and at 855-870 cm.-1 in IV, V, VI, and VII correspond to the 1,2,4-substituted benzene ring and, as they appear in all condensation products, the (CH2)nCOOH radical must be bound in the position 5 or 6 in the I ring system. Maximum absorption frequencies and integral intensities of the stretching vibration C:O bands were determined. The formation of H bonds between NH and C:O bonds affects both the frequency and the intensity of the bands. Two maximum corresponding to the C:O group in COOH and in imidazolone (1665-1685, and 1720-1725 cm.-1, resp.) appear in the spectra of the condensation products. The integral intensities of the 2 CO bands in the condensation products are higher than the sum of CO band intensities in I or II and the corresponding lactone. The increase is explained by the formation of H bonds between the OH of the COOH group and between the C:O group in the 5-membered ring.
IT 1776-93-4 1776-93-8
RL: PRP (Properties)
(spectrum (ir) of, hydrogen bonding and)
RN 1776-93-4 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-2-oxo- (CA INDEX NAME)



RN 1776-93-8 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-1,3-dimethyl-2-oxo- (CA INDEX NAME)

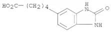
L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1948:2770 CAPLUS
DOCUMENT NUMBER: 42:2770
ORIGINAL REFERENCE NO.: 42:619f-i,620a
TITLE: Ureylene carboxylic compounds
INVENTOR(S): Clapp, Richard C.; Roblin, Richard O., Jr.
PATENT ASSIGNEE(S): American Cyanamid Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

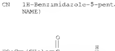
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2418925		19470415	US 1944-546205	19440722

GI For diagram(s), see printed CA Issue.
AB Compds. of the type CONHNHZ-R-CO2H and their salts and esters, where Z is a 6-C ring and R is an alkylene group with 1-6 C atoms, are made, when the ureylene group is in the 3,4-position, by condensing o-phenyleneurea (I) with an aliphatic dicarboxylic acid anhydride with a Friedel-Crafts catalyst, followed by reduction. The 2,3-ureylene compds. are made by chlorinating or sulfonating 2-acylaminophenyl aliphatic acids in the 5-position, then nitrating in the 3-position, hydrolyzing the anilide, reducing the nitro group, removing the Cl or SO3H, and condensing the diamine with COCl2. Cyclohexane derivs. are formed by hydrogenation. I 16, succinic anhydride 12, and AlCl3 64 in (CHCl2)2 600 parts are heated to 100° and finally 120° (total 3 hrs.), then poured into dilute HCl. After steam distillation of the solvent, the γ-keto-γ-(3,4-ureylenephenyl)butyric acid is treated with activated C in NaHCO3 solution, precipitated with acid, and reduced with amalgamated Zn in 18% HCl. γ-(3,4-Ureylenephenyl)butyric acid seps. on cooling. H and PtO2 give the cyclohexyl analog. Similarly δ-(3,4-ureylenephenyl)- and δ-(3,4-ureylenecyclohexyl)valeric acids are made. BzNHC6H4(CH2)3CN is brominated, then nitrated, both in AcOH, hydrolyzed by refluxing with concentrated HCl, and freed from BzOH by evaporation to dryness and extraction with Et2O. Reduction with Na-Mg in NaCO3 solution and passing in COCl2 until strongly acidic precipitated γ-(2,3-ureylenephenyl)butyric acid. δ-(2,3-Ureylenephenyl)valeric acid is made by hydrogenating o-AcNHC6H4CH:CHCH:CHCO2H and proceeding as above. The compds. have bacteriostatic properties.
IT 17767-89-4P, 5-Benzimidazolinevaleric acid, 2-oxo-
RL: PREP (Preparation)
(preparation of)
RN 17767-89-4 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-2-oxo- (CA INDEX NAME)



L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1945:11946 CAPLUS
DOCUMENT NUMBER: 39:11946
ORIGINAL REFERENCE NO.: 39:1846c-i,1847a-e
TITLE: Chemotherapy. IX. Ureylenebenzene and cyclohexane derivatives as biotin antagonists
AUTHOR(S): English, J. P.; Clapp, R. C.; Cole, Q. P.; Halverstadt, I. F.; Lampen, J. O.; Roblin, R. O., Jr
SOURCE: Journal of the American Chemical Society (1945), 67, 295-302
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 39:11946
AB Because a number of important pathogenic organisms probably require preformed biotin and because of the minute quantities present in most body tissues, an investigation of potential biotin antagonists has been carried out. 2-BzNHC6H4(CH2)3CN (2.64 g.) in 20 cc. AcOH, treated with 1.7 g. Br in 5 cc. AcOH during 4 h., gives 96% of γ-(2-benzoylamino-5-bromophenyl)butyronitrile (I) m. 140-1° (m.ps. corrected); 13.8 g. of I in 125 cc. AcOH, treated rapidly with 125 cc. fuming HNO3 in 125 cc. AcOH at about 60° and held at that temperature for 2 h., gives 82% of the 3-NO2 derivative, pale yellow, m. 142-4°; hydrolysis of 1.7 g. by 25 cc. 20% HCl (refluxing 22 h.) gives 58% of γ-(2-benzoylamino-3-nitro-5-bromophenyl)butyric acid (II), m. 167-70°. II (700 mg.) in 80 cc. 5% Na2CO3 (N atmospheric), warmed to 55° and treated with 140 g. 2% Na-Hg during 2.5 h., gives 79% of γ-(2,3-ureylenephenyl)butyric acid (III), m. 299-300°; catalytic reduction (Pt oxide) in AcOH at 50 lb. H pressure for 6 h. gives 2,3-ureylenecyclohexanebutyric acid (IV), separated by fractional acidification from N/7 aqueous KOH with 0.5 N HCl into a fraction m. 218-20°, n1 1.597, n2 1.480, solubility in boiling H2O 15 mg./cc., and a fraction m. 192-4°, n1 1.563, n2 1.536, solubility in boiling H2O 25 mg./cc. Details are given of the synthesis of o-BzNHC6H4CH:CHCH: CHCO2Me (40-65%), o-H2NC6H4CH:CHCH:CHCO2H (69% of the Bz derivative and 73% of the free amine), o-AcNHC6H4CH:CHCH:CHCO2H (83%) and o-AcNHC6H4(CH2)4CO2H (V) (79%), m. 126-8° [Diehl and Einhorn, Ber. 20, 377(1887), gave 151°]. V gives 89% of the 5-Br derivative, m. 152-3°, which yields 88% of the 3-nitro-5-bromo derivative (VI), m. 205-7°; the structure of VI follows from its oxidation to 5,2,3-Br(AcNH)(O2N)C6H2CO2H (also prepared by acetylation of the acid of Adams and Snyder, C.A. 32, 5814.1). VI and 1:1 HCl, refluxed 2.75 h., give 95% of δ-(2-amino-3-nitro-5-bromophenyl)valeric acid, m. 119-21°, which was not purified but was transformed (95% yield) into δ-(2,3-ureylenephenyl)valeric acid (VII), m. 263-5°; this yields 51% of 2,3-ureylenecyclohexane valeric acid (VIII), separated into 2 isomers, m. 222-6°, n average > 1.560, > 1.565, and m. 183°, n average > 1.530, < 1.535. 2,3-Ureylenebenzoic acid (IX) [Griess, Ber. 5, 192(1872)] yields a Me ester, m. 260-3°; catalytic reduction of IX gives 66% of the cyclohexane analog, decomps. 204-5°. 3,4-(H2N)2C6H3CO2H gives 76% of the 3,4-isomer (X) of IX, whose Me ester m. 312-13°; reduction of X gives 45% of the cyclohexane analog, m. 206-7°. o-C6H4(NH)2CO (XI) (1.8 g.) in 175 cc. absolute EtOH and 4 cc. EtOH saturated with HCl, reduced at 45 lb. H pressure and room temperature for 14

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
h., give 38% of hexahydro-o-phenyleneurea, m. 147-9° [Einhorn and Bull, Ann. 295, 209(1897), reported an isomer m. 230-1°]. XI (16 g.), 12 g. succinic anhydride and 630 cc. C2H2Cl4, treated with 64 g. AlCl3 at room temp., heated to 100° during 2.75 h., held at 100-10° for 1 h. and at 110-20° for 0.5 h., give 9% of β-(3,4-ureylenebenzoyl)propionic acid (XIa), m. 294° (decompn.); Clemmensen redn. of XIa (refluxing 5 h.) gives 78% of γ-(3,4-ureylenephenyl)butyric acid (XII), m. 253.5-5°; catalytic redn. of XII gives 43% of the cyclohexyl analog, m. 137-9°. XI (13 g.), 11 g. of glutaric anhydride and 650 cc. C2H2Cl4, treated with 52 g. AlCl3, give 5% of γ-(3,4-ureylenebenzoyl)butyric acid, m. 280-2°; Clemmensen redn. gives 89% of δ-(3,4-ureylenephenyl)valeric acid (XIII), m. 234-6°; the cyclohexyl analog (27%) m. 212-14°. UV absorption spectra are given for VII and IX-XIII. Data are given for the antibiotin activity and mol. inhibition ratios with L. casei and yeast; with the exception of the benzoic acid derivs., all the substances in the present group, both in the benzene and cyclohexane series, proved to be biotin antagonists. Several of the compds. inhibited the growth of L. arabinosus as well, and in all cases the effect could be reversed by appropriate concns. of biotin. None of the products tested showed any growth-promoting activity for any of these organisms. The Ph derivs. were less active than the corresponding cyclohexanes. When L. casei was the test organism, the position of the side chain with respect to the ureylene group seemed to be less important for max. activity than the total no. of C atoms (including the carbocyclic ring) sepg. the ureylene and CO2H groups. With yeast, however, quite the reverse situation was found; the position of the side chain appears to be more significant than the no. of C atoms it contains. There was practically no difference in the antibiotin activity of the 2 isomers of IV and VIII.
IT 17767-89-4P, 5-Benzimidazolevaleric acid, 2,3-dihydro-2-oxo-
36896-35-2P, 5-Benzimidazolevaleric acid, 2,3-dihydro-δ,2-dioxo-
RL: PREP (Preparation)
(preparation of)
RN 17767-89-4 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-2-oxo- (CA INDEX NAME)



RN 36896-35-2 CAPLUS
CN 1H-Benzimidazole-5-pentanoic acid, 2,3-dihydro-δ,2-dioxo- (CA INDEX NAME)

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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